

AN INVITATION TO COMBINATORIAL SPECIES

Federico G. Lastaria
Department of Mathematics, Politecnico di Milano
Milano, Italy

INTRODUCTION

In the last fifty years, a remarkable simplification and unification of mathematics has been achieved through the fundamental concepts of the theory of categories: some familiarity with categorical methods has nowadays become mandatory for everyone interested in twenty-first century mathematics and science.

For instance, the insight of the concepts of category, functor and naturality has provided a proper mathematical foundation to our combinatorial intuition through the notion of *combinatorial species*.

The theory of species, introduced by the Canadian mathematician André Joyal in 1981, simplifies and clarifies the foundations of combinatorics, providing answers to questions that can be roughly phrased as follows.

QUESTION 1. What is a combinatorial structure?

The subtle point in defining a “combinatorial structure” is the following. Let us think of an instance of combinatorial structure, such as the permutations of a set. On the one hand, the specific choice of names - or labels - for the elements of the set is absolutely irrelevant: should we relabel the elements, the permutations themselves would be relabeled accordingly in a natural way. On the other hand, we cannot simply take off the labels: unlabeled permutations, i.e. permutations of indistinguishable objects, are something quite different. In other words, any combinatorial structure, like a graph or a permutation, must be defined without a committed choice of a specific underlying set, but, at the same time, without making the structure itself unlabeled.

Category theory provides the tools to give the proper mathematical definition which is needed: a combinatorial object, or *species*, is a functor from the category **B** of finite sets and bijections to itself. (I will recall the relative definitions in the next section). For instance, the species **Perm** of permutations is the functor that assigns to each finite set E the set $\text{Perm}[E]$ of all the permutations of the set E . To any bijection $f: E \longrightarrow E'$, which may be thought of as a *relabelling* of the elements of E , the rule **Perm** associates a bijection

$$\text{Perm}[f] : \text{Perm}[E] \longrightarrow \text{Perm}[E'] ,$$

the natural *transport* of the permutations along the bijection f . The association $f \mapsto \text{Perm}[f]$ preserves composition of bijections and identities.

Thus the key to grasp the concept of combinatorial structure in mathematical terms consists in using the concept of functor, emphasizing the transport of structures along bijections, rather than the properties of the structures - a point of view already maintained by C. Ehresmann (1965), in contrast with that of the Bourbaki's school. We quote Gian-Carlo Rota (see [1], Foreword):

A labeled graph - or any ‘labeled’ combinatorial construct - is a functor from the groupoid¹ of finite sets and bijections to itself. This definition of a labeled object is not ‘abstract’: on the contrary, it expresses in precise terms the commonsense idea of ‘being able to label the vertices of a graph either by integers or by colours, it does not matter’, and is the only way of making this commonsense idea precise.

To each species M one associates its *exponential generating series*

$$M(x) = \sum_{n \geq 0} a_n \frac{x^n}{n!}$$

Here a_n is the cardinality of $M[E]$, where E is any set with n elements. It has been known at least since Euler that making calculations on generating functions is the essential tool in enumerative combinatorics. Nevertheless, a satisfying *combinatorial interpretation* of formal operations on these series was lacking: all the computational techniques appeared to be a more or less mysterious artisanship. Thus we come to:

QUESTION 2. What combinatorial constructions are we unknowingly performing on species when we make calculations on their generating functions? Otherwise stated, what are the combinatorial interpretations of calculations on formal series?

¹ A *groupoid* is a category all of whose morphisms are invertible.

The theory of species shows how it is possible to define operations with species, i.e. combinatorial constructions, such as sum, product, substitution or derivative in such a way that they naturally correspond to operations on their generating functions. Hence there follows an interplay between combinatorial species and generating functions, reminiscent - roughly speaking - of the interactions between geometry and algebra:

Operations on formal series (in particular, polynomials) with natural coefficients have combinatorial interpretations in terms of species and can be used to solve problems in combinatorics.

According to O. Nava and G.-C. Rota (see [5]):

Generating functions are today what probability distributions were to the early statisticians. What is needed is a new concept which will relate to generating functions much like random variables relate to probability distributions. The missing idea is Joyal's notion of species. With the injection of this fundamental insight, combinatorial intuition can be said to have found a proper foundation.

The aim of this paper is to raise the reader's interest on methods which appear to be rich in educational perspectives. I give only some basic ideas and examples in their simplest setting (saying little about proofs, except to indicate where they can be found). As far as mathematics education is concerned, an introduction to species lends itself to the opportunity of remarking the following themes, listed in order of increasing generality and importance:

1. The conceptual insight of species and their operations, enriched with the use of pictures, simplifies our understanding of the combinatorial constructions and can suggest what calculations need to be done, thus providing an instance of interplay of conceptual, visual and computational aspects in mathematics.
2. Much of the usefulness of mathematics, in the field of education and even in that of applications, stems from finding good conceptual definitions (much more than just "precise" ones).
3. One of the plagues of mathematical education is teaching tricks instead of concepts. Tricks are readily forgotten and are altogether irrelevant, for mathematicians as well as for everybody who makes use of mathematics. With the welcome advent of technology, some of the old repertoires of ad-hoc techniques too often practiced in the teaching of mathematics, even at an advanced level, are at last becoming more and more obsolete, useless and pathetic. As a matter of very survival, in order to characterize the specific role and *raison d'être* of their discipline (as well as for justifying requests of research funds), mathematicians should pay paramount attention also in analyzing, learning and teaching general and pervasive concepts and methods - like those of category theory - that can be used in different fields as a guide to organize and improve mathematical knowledge and its applications (see [3]).

1. COMBINATORIAL SPECIES

The term "combinatorial" originates from the treatise *De arte combinatoria*, an essay on philosophy and logic written by G.W. Leibniz in 1666 at the age of twenty. From its very beginning, combinatorics is more than counting: it is the art of combining objects, and concepts, together.

Now *what are the objects that are being combined? Otherwise stated, what is the definition of combinatorial structure?*

Definition of species

A species is a functor $M : \mathbf{B} \longrightarrow \mathbf{B}$ from the category \mathbf{B} of finite sets and bijections to itself.

Explicitly, a species M assigns:

- To each finite set E , a finite set $M[E]$, called the set of *structures* of species M on E , or the set of M -structures;
- To each bijection f from a set E to a set E' , a bijection $M[f] : M[E] \longrightarrow M[E']$, called the *transport* of the M -structures along f ,

in such a way that:

- (M preserves composition) For all bijections $f : E \longrightarrow E'$ and $g : E' \longrightarrow E''$, the following equality holds:

$$M[gf] = M[g] M[f]$$

(First apply $M[f]$, then $M[g]$).

- (M preserves the identities) For every finite set E ,

permutations. We clearly recognize that the construction which consists in considering all the permutations of a given set E is essentially independent of the assignment of a specific set of labels for its elements. More precisely, saying that constructing the permutations of E is 'independent of the nature' of the elements of E simply means that for any bijection $f : E \longrightarrow E'$, viewed as a *relabelling* of the elements of E by means of the elements of E' , a bijection $\text{Perm}[E] \longrightarrow \text{Perm}[E']$ is defined accordingly in an obvious way. The definition of species as a functor is the precise mathematical rendering of this idea.

Sometimes, even unconsciously, one exploits the irrelevance of the nature of the elements by choosing once and for all a standard privileged set, typically the set of integers $\{1, \dots, n\}$. Such a seemingly innocent choice stealthily sneaks the idea of linear order, which may turn out to be misleading (For example, it confuses linear orders with permutations).

Recall that the exponential generating series of a species M is $M(x) = \sum_{n \geq 0} a_n \frac{x^n}{n!}$, where a_n is the cardinality of $M[E]$,

E being any set with n elements.

EXAMPLES OF SPECIES AND THEIR GENERATING SERIES.

1) The species Lin of linear orders ($\text{Lin}(E)$ is the set of all the linear orders on the set E). Its generating series is $\text{Lin}(x) = 1 + x + x^2 + x^3 + \dots + x^n + \dots = (1-x)^{-1}$. (Note that the species Perm and Lin have the same generating series).

2) The uniform species U , which associates to every set E the singleton $\{1_E\}$, the identity of E . One can interpret this species as assigning to each set E the unique set structure on E . Its exponential generating function is the exponential series: $U(x) = \exp(x)$.

3) The species T of trees (connected acyclic graphs). One proves that $T(x) = \sum n^{n-2} x^n / n!$

(See further, Cayley's theorem).

As an added bonus, note that once a species is defined as an endofunctor of the category \mathbf{B} of finite sets and bijections, the crucial notion of isomorphism of species, i.e. the mathematical rendering of the idea of species “being the same”, comes for free: isomorphisms are invertible natural transformations. We recall some general definitions and will be more explicit on this point.

Natural isomorphism

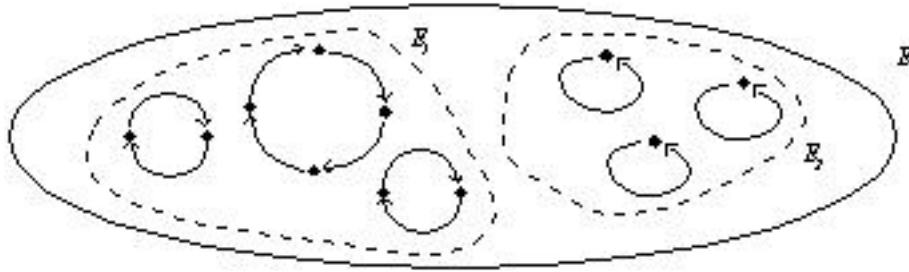
If M and N are two species of structures, a *natural isomorphism* $\mathbf{I} : M \longrightarrow N$ consists of a family of bijections $\mathbf{I}_E : M[E] \longrightarrow N[E]$, one for every set E , which are *natural* in the following sense: for every bijection $f : E \longrightarrow F$, the following commutativity condition holds:

$$\mathbf{I}_F \circ M[f] = N[f] \circ \mathbf{I}_E$$

Interpret \mathbf{I}_E as a construction which, given any structure s of species M on the set E produces a structure $\mathbf{I}_E(s)$ of species N on the same set E . Then, saying that the construction \mathbf{I} is natural, or equivariant, means informally that it does not change when the input and the output are changed simultaneously along the same bijection. Otherwise stated, bijections are natural when they are “intrinsic”, in the sense that they do not depend on coordinate systems introduced by arbitrary enumerations. Note that the species Perm of permutations and the species Lin of linear orders are not isomorphic, i.e. there is no natural isomorphism between them (consider sets with exactly two elements), even though they are equipotent, i.e. they have the same generating series.

2. PRODUCT OF SPECIES

DERANGEMENTS. Let us see how the species of permutations can be expressed as the product of two other species. Look at the internal diagram of a permutation of a set E :



We distinguish two (possibly empty) disjoint subsets whose union is E :

- a set E_1 of points that belong to cycles of length at least two, i.e. a set of points along with a structure of a *derangement* (permutation without fixed points) on it;
- the complementary set E_2 which consists of all the fixed points, i.e. a set together with the (unique) structure of set that it supports.

We say that the species Perm of permutations is the product of the species Der of derangements and the species U of sets and write

$$\text{Perm} = \text{Der} \cdot \text{U}$$

Passing to the exponential generating functions, one has: $(1-x)^{-1} = \text{Der}(x) \exp(x)$. Hence:

$\text{Der}(x) = \exp(-x) (1-x)^{-1}$. Expanding this exponential generating series as $\sum D_n x^n / n!$ we

obtain the number D_n of derangements of a set with n elements:

$$D_n = (1 - 1 + 1 \cdot 2! - 1 \cdot 3! + 1 \cdot 4! - \dots + (-1)^n n!) n!$$

Note that $D_n/n! \rightarrow e^{-1}$ when n goes to infinity, which gives a well known probabilistic interpretation of the inverse of the Napier's constant e (and suggests a way to define it).

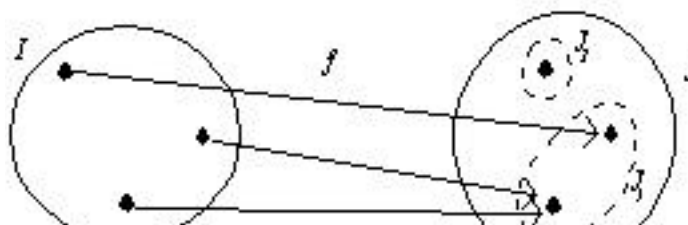
Product of Species

A *decomposition* of a set E into two *parts* is an ordered pair (E_1, E_2) of (possibly empty) disjoint subsets of E whose union is E . If (E_1, E_2) is a decomposition of E , we write $E = E_1 + E_2$. Recall that the order of the summands matters. The *product* $F \cdot G$ of two species is the species defined as follows: for any finite set E , an element of $(F \cdot G)[E]$ is a decomposition $E = E_1 + E_2$ together with an F -structure on E_1 and a G -structure on E_2 . Transport of structures is defined in the obvious way. Informally, an $(F \cdot G)$ -structure is an ordered pair formed by an F -structure and a G -structure over complementary disjoint subsets.

One defines the product of n species in a similar way. One easily proves (see [6]) that the product of species corresponds to the product of their generating functions:

$$(F \cdot G)(x) = F(x) \cdot G(x)$$

THE SURJECTIVE FUNCTIONS. Counting the surjective functions from a set with m elements to a set with n elements is by no means easy. The operation of product of species provides an elegant solution as



follows. Let I be a fixed set with m elements. For lack of a better notation, denote by Epi the species which associates to every set J the set $\text{Epi}(I, J)$ of surjective functions from I to J and by Set the species which associates to any set J the set of all functions from I to J (with the obvious transports of structures). Let $f: I \longrightarrow J$ be an arbitrary function and let J_1 be its image:

The function f consists of the following assignment:

- 1) a surjective function $f: I \longrightarrow J_1$, i.e. an Epi-structure on J_1 ;
- 2) a structure of set on the complementary subset $J_2 = J \setminus J_1$, i.e. a U-structure on J_2 .

Thus:

$$\text{Set} = \text{Epi} \cdot \text{U}$$

Passing to the generating functions:

$$\sum_{n \geq 0} n^m \frac{x^n}{n!} = \left(\sum_{n \geq 0} E_{m,n} \frac{x^n}{n!} \right) \exp(x)$$

where $E_{m,n}$ is the number of surjections from a set with m elements to a set with n elements. Multiplying by $\exp(-x)$, with some calculations we get the answer:

$$E_{m,n} = \sum_{k=0}^n \binom{n}{k} (-1)^k (n-k)^m$$

3. PROBLEMS AND TECHNOLOGY

The use of technology in the teaching of mathematics is a controversial one. In Italy at the high school final examinations (the so called “maturità” exams), graphic and symbolic calculators are forbidden, possibly on the ground that they are an unfair instrument which makes it impossible to judge the students’ mathematical maturity. Some mathematicians fear the negative influence of technology on mathematics in general, and on its teaching in particular.

The threat all mathematicians should react to is teaching tricks instead of emphasizing the fundamental concepts. A great deal of excellent mathematics can be taught by exploiting the interaction between conceptual and technological aspects.

As far as this point of view is concerned, combinatorics is a somewhat neglected field. Students should be taught that when they make calculations on formal polynomials (or series) with natural coefficients, they are actually solving problems in combinatorics unknowingly. Asking a student to solve combinatorial problems insisting both on the use of species and on the use of symbolic calculators, can turn out to be an effective way of practicing good mathematics.

PROBLEM 1. Find the number of ways in which one can distribute four identical objects into five ordered boxes with at most one object in each of the first three boxes and at most two in the last two boxes.

A good answer, from both the conceptual and the computational viewpoint, is the following: the number is the coefficient of x^4 in the expansion of the polynomial

$$(1+x)^3 (1+x+x^2)^2.$$

Explaining the answer and making appropriate generalizations (what about distinguishable objects?) is a good piece of mathematics. (We multiply five species and consider their *ordinary* generating functions, which reflects the requirement that the objects are indistinguishable.)

A more difficult problem is the following.

PROBLEM 2. Count all ways of placing h distinguishable flags on n distinguishable flagpoles. Any number of flags can be placed on each flagpole and the order of flags on each flagpole matters.

First solution. The problem may be solved by an ad-hoc argument. You have n choices of a flagpole for the first flag. If flag 2 is on the same flagpole as flag 1, then you can place it above or below flag 1, otherwise you can choose any of the remaining $n-1$ flagpoles. Thus we have $n+1$ choices for flag 2. Similarly we have $n+2$ choices for flag 3 and in general $n+k-1$ choices for flag k . Thus the answer to the problem is the upper factorial $n(n+1) \cdots (n+k-1)$ (the number of *multisets* with k elements of a set with n elements).

Second solution. A more general and conceptual way to attack the problem consists in thinking in terms of operations on species, as follows. We have a set E of h flags and a set S of n flagpoles. Placing the flags on the flagpoles, taking the order on every flagpole into account, amounts to performing the following items:

- Fixing an ordered n -tuple (E_1, \dots, E_n) of (possibly empty) disjoint subsets of E whose union is E .
- Here E_j is the subset of flags placed on flagpole j ;
- Endowing each part E_j with a linear order structure.

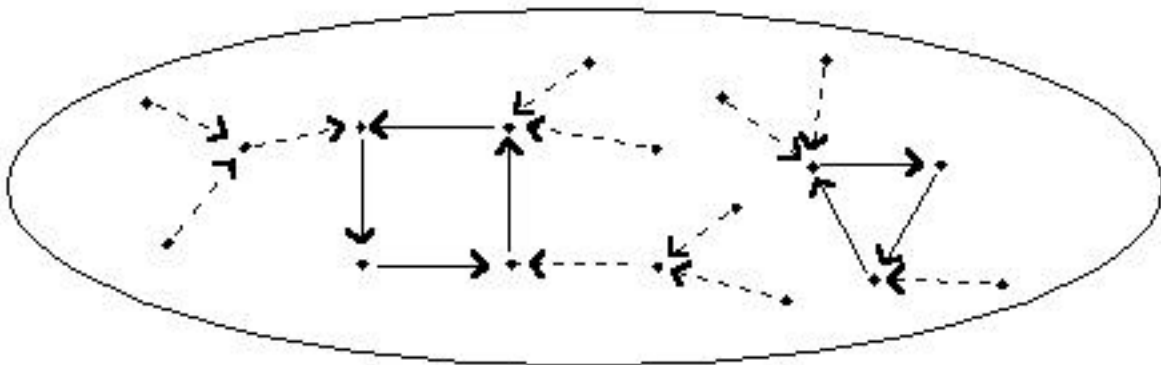
Recalling the definition of product of species, we see that the combinatorial construction hidden in the word problem above can be made explicit: we are asked to count the number of structures of the product species $\text{Lin} \cdots \text{Lin} = \text{Lin}^n$ on the set E . Since the exponential generating function of the species Lin is $(1-x)^{-1}$, the exponential generating function of the species Lin^n is $(1-x)^{-n}$. Thus the solution to our problem is the coefficient of x^h $h!$ in the expansion of $(1-x)^{-n}$. Recalling the generalized Newton's binomial theorem, we find again the upper factorial $n(n+1) \cdots (n+k-1)$. (I have put some calculations under the rug).

4. COMBINATORIAL SUBSTITUTION OF SPECIES

Combinatorial substitution of species, corresponding to the functional composition of generating functions, is the most remarkable application of the definition of species.

MOTIVATING EXAMPLE: ENDOMAPS. Consider the internal diagram of an endomap

$f: E \rightarrow E$ of a finite set E , that is the directed graph consisting of the elements of E as vertices, with one arrow from x to $f(x)$ for every x in E (E has 18 elements in the picture below).



If we repeatedly apply f to an element of E , we eventually enter a cycle (in the picture, the square and the triangle), since the set E is finite. Call the points on these cycles *periodic* points. Each periodic point r is the root of a tree whose vertices are the elements of E which enter a cycle for the first time at r , under repeated applications of f . In our example there are seven periodic points and therefore seven rooted trees, whose edges are dashed (Two of these rooted trees consist only of their root). The endofunction f permutes the periodic points and therefore permutes the set of rooted trees as well. Thus the figure shows that *any endofunction can be naturally identified with a permutation of disjoint rooted trees*. We recall that naturality means, intuitively, that the way of constructing a permutation of rooted trees starting from an endofunction does not depend on the specific names of the elements of the underlying set. Conversely, given a family of rooted trees along with a permutation of this family, the figure suggests the way of recovering the corresponding endofunction in an obvious way.

In the language of species we say that the species Endo of endofunctions is obtained by *substitution*² of the species A of rooted trees in the species Perm of permutations and write

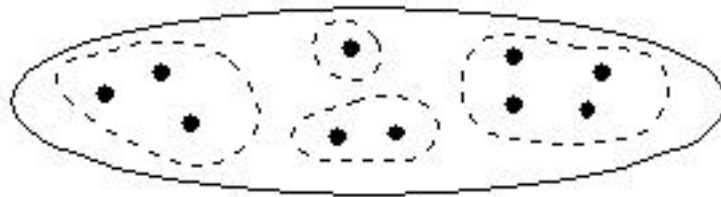
$$\text{Endo} = \text{Perm}(A)$$

A striking application of this combinatorial identity will be shown shortly (Cayley's theorem).

To summarize, an endomap of a set E consists of the following data:

- a partition \mathbf{p} of E (each block is the set of the vertices a rooted tree);
- an A-structure, i.e. a structure of rooted tree, on every block of \mathbf{p} ;
- a Perm-structure, i.e. a permutation, on the set of the blocks of \mathbf{p} .

SECOND EXAMPLE: PARTITIONS OF A SET. Consider the species Part of partitions, that is the species which associates to every finite set E the set of all partitions of E . Every partition of a set E is a set of nonempty disjoint subsets of E :



Thus we have the combinatorial identity $\text{Part} = \text{U}(\text{U} - 1)$, where U denotes the uniform species (the species of sets) and $\text{U} - 1$ is the species of nonempty sets. Passing to generating series yields

$$\text{Part}(x) = \exp(\exp x - 1) = \sum_{n \geq 0} B_n \frac{x^n}{n!}.$$

Thus the number B_n of partitions of a set with n elements is the coefficient of $x^n/n!$ in the expansion of the function $\exp(\exp x - 1)$. The B_n 's are the so called *Bell numbers*.

AN APPLICATION: COUNTING TREES (CAYLEY'S THEOREM) As an application of the substitution of species, we now give an elegant proof, due to A. Joyal (see [2]), of Cayley's theorem: the number t_n of labeled trees on a set of n elements ($n \geq 1$) is $t_n = n^{n-2}$. Given any tree, choose an ordered pair of (not necessarily distinct) vertices, say (t, h) , the *tail* and the *head*. What you get is a *vertebrate*. Denote by v_n the number of vertebrates on a set with n elements ($n \geq 1$). Since a pair of distinguished vertices (t, h) may be chosen in n^2 in different ways, we have $v_n = n^2 t_n$. The shortest path from the tail t to the head h of a vertebrate is the *vertebral column*. The vertices in linear order, from the tail t to the head h on the vertebral column are the *vertebras*. For each vertex p of the vertebrate, let $v(p)$ be the vertebra which is closest to p . Each fibre of the function v has a structure of rooted tree, the root being the vertebra. Thus a vertebrate on a set E consists of:

- a partition \mathbf{p} of E into non-empty blocks ;
- a structure of rooted tree on each block of the partition;
- a (non-empty) linear order on the partition \mathbf{p} .

Thus the species Vert of vertebrates is obtained by substitution of the species A of rooted trees in the species Lin_+ of nonempty linear orders :

$$\text{Vert} = \text{Lin}_+(A)$$

² In probability theory, the operation of substitution occurs in the theory of branching processes.

In short, a vertebrate is an ordered set of rooted trees. We already know that an endofunction is a permutation of rooted trees. Now, the species Lin and Perm are equipotent (i.e., they have the same number of structures on any n -set, namely $n!$). Therefore on any nonempty n -set there are equally many vertebrates and endofunctions, i.e. $v_n = n^n$. Recalling that $v_n = n^2 t_n$, we conclude that $t_n = n^{n-2}$, the classic formula for the number of labeled trees (Cayley, 1859).

Substitution of species

Given two species F and G such that $G[\emptyset] = \emptyset$, the *substitution* of G into F is the species $F(G)$ defined as follows: an $F(G)$ -structure on a set E consists of a triplet $(\mathbf{p}, \mathbf{g}, \mathbf{j})$, where:

- \mathbf{p} is a partition of E ;
- $\mathbf{g} = (\mathbf{g}_p)_p$, where each \mathbf{g}_p is a G -structure on the set p ;
- \mathbf{j} is an F -structure on the set of blocks of \mathbf{p} .

The transport of structures for $F(G)$ is naturally induced by the transport of structures of F and G . One easily proves (see [6]) that the exponential generating series of the species $F(G)$ satisfies the equality of formal series:

$$(F(G))(x) = F(G(x))$$

One cannot substitute the series $G(x)$ into the series $F(x)$ unless $G(x)$ has no constant term. This explains why one requires $G[\emptyset] = \emptyset$.

ACKNOWLEDGMENTS: To Gian-Carlo Rota - in memory - from whom I have learnt that one can do mathematics putting colored marbles into boxes.

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Federico G. Lastaria
 Department of Mathematics, Politecnico di Milano
 Piazza Leonardo da Vinci 32, 20133 Milano, Italy
 e-mail address: fedlas@mate.polimi.it